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Calculation of Time-Dependent Heat Flow in a Thermoelectric Sample

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CALCULATION OF TIME-DEPENDENT HEAT FLOW IN A THERMOELECTRIC SAMPLE

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Abstract

In this project, the time-dependent one-dimensional heat equation with internal heating is solved using eigenfunction expansion, according to the thermoelectric boundary conditions. This derivation of the equation describing time-dependent heat flow in a thermoelectric sample or device yields a framework that scientists can use (by entering their own parameters into the equations) to predict the behavior of a system or to verify numerical calculations. Allowing scientists to predict the behavior of a system can help in decision making over whether a particular experiment is worthy of the time to construct and execute it. For experimentalists, it is valuable as a tool for comparison to validate the results of an experiment. The calculations done in this derivation can be applied to pulsed cooling systems, the analysis of Z-meter measurements, and other transient techniques that have yet to be invented. The vast majority of the calculations in this derivation were done by hand, but the parts that required numerical solutions, plotting, or powerful computation, were done using *Mathematica 8*. The process of filling in all the steps needed to arrive at a solution to the time-dependent heat equation for thermoelectrics yields many insights to the behavior of the various components of the system and provides a deeper understanding of such systems in general.

Keywords: thermoelectrics, transient heat equation, Z-meter, pulsed cooling, dynamic heat flow.

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1. Introduction

1.A Thermoelectric Materials

Thermoelectric materials are materials that have significant thermoelectric properties; i.e. materials that convert a temperature gradient into an electrical current (the Seebeck effect), an electric current into a temperature gradient (the Peltier effect), and either absorb or emit heat as current flows through them when there is a temperature difference between that material's ends (the Thomson effect). Together, these three phenomena are known as the thermoelectric effect [6]. The most effective thermoelectric materials are semiconductors. The relative worth of a thermoelectric material is given by its "figure of merit," Z. Z is given by the equation:

$$\textbf{(1.1)}\ Z = \frac{S^2 \sigma}{K}$$

where σ is the electrical conductivity, S is the Seebeck coefficient, and K is the thermal conductivity. A greater Z indicates greater thermoelectric efficiency.

Thermoelectrics are important because they have properties that allow them to serve as power generators and refrigerators in applications where traditional generators and refrigerators are prohibited due to their size or need for maintenance. They can be miniaturized and are used extensively in temperature sensors in both scientific measuring devices and temperature control systems [6]. One application of thermoelectrics that matters much today due to current global concern about energy and the environment is that thermoelectric devices (TEDs) can be used for energy harvesting, in which wasted thermal energy from processes such as power generation can be captured and turned into electrical power. One particularly fascinating example of thermoelectric power generation is the Voyager I spacecraft which uses a Radioisotope Thermoelectric Generator (RTG) that operates by turning the temperature gradient (generated by the heat produced by 24 pressed plutonium oxide spheres and the coldness of space) into electricity. The electricity powers the equipment on board the spacecraft which, after over 34 years, still sends scientific data about its surroundings through the Deep Space Network [9]. Additionally, thermoelectric devices can perform cyclic temperature changes and are reliable in doing so, which allows them to be used in polymerase chain reaction (PCR) applications which are used in DNA analysis. Another use of cyclic thermoelectric cooling is its incorporation into mid-infrared laser gas sensors, in which the accuracy of measurement is improved by the thermoelectric cooler's momentary cooling capability [2]. Thermoelectrics have numerous applications, and more are being discovered.

We study thermoelectrics to discover new and more effective ways in which to use them and because we hope to make better TEDs. Creating more effective TEDs can be achieved by creating thermoelectric materials that have favorable characteristics (e.g. high electrical conductivity (σ), low thermal conductivity (K), and a high Seebeck coefficient (S)) so they will be more efficient [9].

1.B Applications of Dynamic (Time-Dependent) Heat Flow in a Thermoelectric Device or Material

1.B.i Pulsed Cooling

In a pulsed cooling system, a thermoelectric device is operated with the optimal amount of (constant) current required to achieve its maximum level of steady-state Peltier cooling. Then an additional pulse of current is applied to increase, for a brief moment, the amount of cooling that the device can accomplish. The additional current does cause increased Joule heating throughout the device so the whole device will increase in temperature, but the additional cooling caused by the Peltier effect occurs instantaneously at the cold side, momentarily boosting the cooling capacity of the device before the heat caused by the Joule heating can affect the cold side [1]. Joule heating is the generation of heat caused by the moving particles that form the current interacting with other particles in the conductor, and heat generated this way takes time to diffuse throughout the material. Devices that accomplish refrigeration by the pulsed cooling method are usually in contact with whatever they are cooling only during the coldest part of their operation. Even during the steady-state operation of a thermoelectric cooler, both Joule heating and the Peltier effect are in play: The maximum steady-state cooling is the coldest temperature that device can achieve while overcoming the heat generated by the current running through the device.

1.B.ii Z-Meter

In order to directly measure the thermoelectric figure of merit, Z, the two components of voltage, the resistive component and the Seebeck component, must be distinguished from one another. This is because the measurement of the Seebeck voltage, which is caused by thermo-electric effects, can be used to characterize the material's thermoelectric properties. In a Z-meter setup, the thermoelectric sample has a direct current (DC) flowing through it, which causes a temperature gradient across the sample due to the Peltier effect. The temperature difference between the ends in turn generates a Seebeck voltage. When the current is turned off, the electrical (resistive) voltage disappears instantly, but the Seebeck voltage drops off slowly because of the heat dissipation and heat capacity of the materials and can be measured at the instant the current is removed [4].

1.C Heat Transfer

Conduction is the primary form of heat transfer in the processes detailed in this project. In a semiconductor, heat is transferred primarily by two processes: energy flow due to vibrations of the crystal lattice and energy carried by the charge carriers (electrons and/or holes). The term hole describes the lack of an electron at a position where one could exist. In addition to the transfer of heat, the electrical current (movement of free electrons or, in some cases, holes) is responsible for the generation of the temperature gradient resulting from the Peltier effect. Whether it is electrons or holes that move throughout the material depends on what type of material it is. All semiconductors have both electrons and holes moving about, but one is in the majority so typically only one is considered. In an open circuit system (one in which no current is flowing), the diffusion of the electrons (or holes) from the hot side to the cold side of the thermoelectric material causes a thermoelectric voltage because the migrating charge carriers leave behind their oppositely charged atomic core. This creates an electric potential called the Seebeck potential. The magnitude of this effect is characterized by the Seebeck coefficient (S), which is typically measured in μV/K:

(1.2) $$S = \frac{V}{\Delta T}$$

where V is the voltage in Volts and ΔT is the temperature in Kelvins between the two ends of the material. The potential difference (V) is given by:

(1.3) $$V = S\Delta T$$

The Peltier effect, characterized by the Peltier coefficient (Π), is related to the Seebeck effect by :

(1.4) $$\Pi = ST$$

2. Derivation

2.A Problem

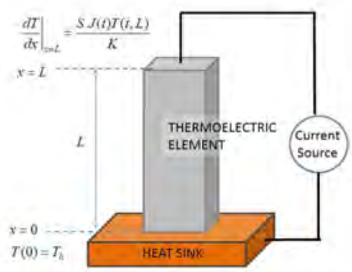

Figure 1. Description of the system. A thermoelectric element is attached to a heat sink held at constant temperature. A current source drives an electrical current through the element causing the opposite side to cool.

The problem is to solve for the time-dependent heat transport of the thermoelectric material shown in Figure 1.

2.B Definition of symbols:

$T(x, t)$ – temperature

$J(t)$ – current density

x – position variable

t – time variable

L – total length of thermoelement

T_h – hotside temperature

S – Seebeck coefficient

K – Thermal conductivity

h – $\frac{S\,J}{K}$

2.C Partial Differential Equation with Boundary Conditions

T(x,t) means the temperature measured at position x and at time t. As an example, T(10,4) would mean the temperature 10 units of length, e.g. 10 μm from the end of the sample, after four units of time, e.g. four seconds, have elapsed.

Boundary conditions (BCs) are the conditions at the ends of the sample (when x=0 and x=L). L is a symbol for maximum length and is a number with units of length such as micrometers (μm). Alternatively, L=1 (L equals one) can express maximum length, using the convention of giving x as a fraction of the sample's total length. In this case, T(0.5,4) would mean the temperature halfway down the sample after four seconds have elapsed.

The initial condition (IC) is the description of the state of the system at the start of the experiment or process (when t=0). In this case, the IC is the temperature at the start of the experiment.

The partial differential equation which describes the one dimensional flow of heat through the sample, as well as the generation of heat within the sample is given by [1], [5]

$$\textbf{(2.1)}\; a \frac{\partial^2 T(x,t)}{\partial x^2} + \frac{J^2(t)\, a}{K\,\sigma} = \frac{\partial T(x,t)}{\partial t}$$

Solution of this equation gives the temperature T as a function of position (x) and time (t). In Eq. (2.1), a is the thermal diffusivity, K is the thermal conductivity, σ is the electrical conductivity, and J is the electrical current density. The additional term, $\frac{J^2(t)\,a}{K\,\sigma}$, describes the internal heating of the sample due to the current flowing through it.

Equation (2.1) is subject to the boundary condition,

$$\textbf{(2.2)}\; K \left.\frac{dT}{dx}\right|_{x=L} = -S\,T(L,t)\,J$$

This means that the heat flux at the x=L boundary is equal to the Peltier coefficient, Π=ST, multiplied by the current density, J. The boundary condition at the x=0 boundary is a restriction on the temperature at that boundary,

(2.3) $T(0,\ t) = T_h$

We choose the initial temperature to be the same throughout the whole sample, and we will name it for the side which is heat sunk (x=0), which will be the hot side when the system is on, hence the name T_h. The initial condition is:

(2.4) $T(x,\ 0) = f(x) = T_h$

The solution to Eq. (2.1) subject to the boundary conditions Eqs. (2.2) and (2.3) and initial condition Eq. (2.4), follows that of Zhou, 2007. Following Zhou, we construct a function r(x).

(2.5) $r(x) = T_h \left(1 - \frac{x}{L}\right)^2$

This function, r(x), is the description of the behavior the system during steady-state operation. We define a new function v(x,t)

(2.6) $v(x,\ t) = T(x,\ t) - r(x)$

The function, v(x,t), is the description of the transient behavior of the system, e.g. when an additional pulse of current is applied.

Because we are interested in the transient behaviour of the system, we will rearrange Eq. (2.6) such that

$T(x,\ t) = v(x,\ t) + r(x)$

and substitute it into (2.1), which will ultimately allow us to isolate the transient part of the solution:

$$\textbf{(2.7)} \qquad a \frac{\partial^2 (v(x,\ t) + r(x))}{\partial x^2} + \frac{J^2 a}{\mathrm{K}\,\sigma} = \frac{\partial (v(x,\ t) + r(x))}{\partial t}$$

Expanding,

$$\textbf{(2.8)} \qquad a \frac{\partial^2 v(x,\ t)}{\partial x^2} + a \frac{\partial^2 r(x)}{\partial x^2} + \frac{J^2 a}{\mathrm{K}\,\sigma} = \frac{\partial v(x,\ t)}{\partial t} + \frac{\partial r(x)}{\partial t}$$

The last term equals zero because r(x) is not a function of time yielding

$$\textbf{(2.9)} \quad a \frac{\partial^2 v(x,\ t)}{\partial x^2} + a \frac{\partial^2 r(x)}{\partial x^2} + \frac{J^2 a}{\mathrm{K}\,\sigma} = \frac{\partial v(x,\ t)}{\partial t}$$

Now take the derivative of r(x) twice with respect to x.To simplify the process of differentiating r(x), expand the Eq. (2.5),

$$\textbf{(2.10)}\ r(x) = T_h - \frac{2\,T_h\,x}{L} + \frac{T_h\,x^2}{L^2}$$

Taking the first derivative yields,

$$\textbf{(2.11)}\ \frac{d\,r(x)}{d\,x} = \frac{d}{d\,x}\left(T_h - \frac{2\,T_h\,x}{L} + \frac{T_h\,x^2}{L^2}\right) = 0 - \frac{2\,T_h}{L} + \frac{2\,T_h\,x}{L^2}$$

Taking another derivative yields,

$$\textbf{(2.12)}\ \frac{d}{dx}\left(-\frac{2\,T_h}{L}+\frac{2\,T_h\,x}{L^2}\right)=0+\frac{2\,T_h}{L^2}$$

Therefore,

$$\textbf{(2.13)}\ \frac{d^2 r(x)}{dx^2}=\frac{2\,T_h}{L^2}$$

Substituting this into Eq. (2.9) yields the partial differential equation (PDE) for v(x,t)

$$\textbf{(2.14)}\ a\,\frac{\partial^2 v(x,\,t)}{\partial x^2}+Q=\frac{\partial v(x,\,t)}{\partial t}$$

where

$$\textbf{(2.15)}\ Q=\frac{2\,a\,T_h}{L^2}+\frac{J^2\,a}{\mathrm{K}\,\sigma}$$

After having substituted the expression of T(x,t) that is composed of a transient component and a steady-state component into the one-dimentional heat equation, the BCs for the transient component, v(x,t), are

$$\textbf{(2.16)}\ v(0,\,t)=0$$

$$\textbf{(2.17)}\ \left.\frac{\partial v}{\partial x}\right|_{x=L}=-\frac{S\,J\,v(L,\,t)}{\mathrm{K}}$$

and the initial condition is,

$$\textbf{(2.18)}\ v(x,\,0)=f(x)-r(x)=g(x),$$

Notice here that $f(x)=T_h$.

Substituting the expanded form of r(x) into g(x), we get a more simplified form:

$$\textbf{(2.19)}\ g(x)=f(x)-r(x)=T_h-\left(T_h-\frac{2\,T_h\,x}{L}+\frac{T_h\,x^2}{L^2}\right)=\frac{2\,T_h\,x}{L}-\frac{T_h\,x^2}{L^2}$$

Which after factoring out T_h, g(x) is expressed as the even simpler expression:

$$\textbf{(2.20)}\ g(x)=T_h\left(\frac{2\,x}{L}-\frac{x^2}{L^2}\right)$$

This result will be used later in an integral in Eq. (2.73).

Now that the BCs and the IC of Eq. (2.14) have been addressed, we solve Eq. (2.14) by the eigenfunction expansion method [1]. (The choice of this method is vindicated by an exercise in Appendix C.) The eigenfunction expansion method is a typical method used to solve such PDEs, and the eigenfunctions are obtained from the corresponding homogeneous PDE, which is obtained from Eq. (2.14) by setting Q=0,

$$\textbf{(2.21)}\ a\,\frac{\partial^2 v(x,\,t)}{\partial x^2}=\frac{\partial v(x,\,t)}{\partial t}$$

To determine a solution, we assume that v(x,t) can be written with its variables separated such that:

$$\textbf{(2.22)}\ v(x,\,t)=G(t)\,\varphi(x)$$

Substituting (22) into (21):

$$(2.23)\ a\ \frac{\partial^2}{\partial x^2}(G(t)\,\varphi(x)) = \frac{\partial}{\partial t}(G(t)\,\varphi(x))$$

Switching from Leibniz's notation to Lagrange's notation for ease of reading:

$$(2.24)\ a\,G(t)\,\varphi''(x) = G'(t)\,\varphi(x)$$

Rearranging to get all functions of t on the left and all functions of x on the right:

$$(2.25)\ \frac{G'(t)}{a\,G(t)} = \frac{\varphi''(x)}{\varphi(x)}$$

Since x and t are variables that are independent of one another, the two ratios in the above equation must be constant. Thus,

$$\frac{G'(t)}{a\,G(t)} = c \ \text{ and } \frac{\varphi''(x)}{\varphi(x)} = c.$$

We can write the the constant, originally expressed as c, as -λ in order to denote that the values of c are eigenvalues of the equation. An eigenvalue is a member of a set of values of a parameter for which a differential equation has a nonzero solution under given conditions.

$$(2.26)\ \frac{G'(t)}{a\,G(t)} = \frac{\varphi''(x)}{\varphi(x)} = -\lambda$$

Going back to Leibniz's notation, we arrive at

$$(2.27)\ \frac{1}{a\,G(t)}\,\frac{dG(t)}{dt} = \frac{1}{\varphi(x)}\,\frac{d^2\varphi(x)}{dx^2} = -\lambda$$

The spatial equation (the x-dependent part) is:

$$(2.28\,a)\ \frac{1}{\varphi(x)}\,\frac{d^2\varphi(x)}{dx^2} = -\lambda$$

or

$$(2.28\,b)\ \frac{d^2\varphi(x)}{dx^2} = -\lambda\,\varphi(x)$$

$$(2.28\,c)\ \frac{d^2\varphi(x)}{dx^2} + \lambda\,\varphi(x) = 0$$

And the boundary conditions are:

$$(2.29\,a)\ \varphi(0) = 0$$

$$(2.29\,b)\ \frac{d\varphi(L)}{dx} = -\frac{S\,J\,\varphi(L)}{\mathrm{K}}$$

noting that x=0 is the side of the sample that is at ambient temperature, T_h. $\varphi(0)=0$ is simply the expression of the fact that the transient temperature v(x,t)=0 at that boundary, x=0, as shown in Eq. (2.16). The calculation then is seen as a calucation of the change in temperature (ΔT). Since we are dealing only with the spatial equation there is no IC.

To solve Eq. (2.29), assume a solution will be proportional to $e^{\gamma x}$ for some constant γ.

Substitute $\varphi(x)=e^{\gamma x}$ into (2.28c):

$$(2.30)\ \frac{d^2 e^{\gamma x}}{dx^2} + \lambda\,e^{\gamma x} = 0$$

Now make the substitution of $\frac{d^2}{dx^2}(e^{\gamma x}) = \gamma^2 e^{\gamma x}$ into (2.30):

(2.31) $\gamma^2 e^{\gamma x} + \lambda e^{\gamma x} = 0$

Factor out $e^{\gamma x}$:

(2.32) $(\lambda + \gamma^2) e^{\gamma x} = 0$

Since $e^{\gamma x} \neq 0$ for any finite γ, the zeros must come from the polynomial:

(2.33) $\lambda + \gamma^2 = 0$

Solve for γ:

$\gamma = i\sqrt{\lambda}, \quad \gamma = -i\sqrt{\lambda}$

The root $\gamma = -i\sqrt{\lambda}$ gives

(2.34) $\varphi_1(x) = c_1 e^{-i\sqrt{\lambda}\, x}$

as a solution, where c_1 is an arbitrary constant.

The root $\gamma = i\sqrt{\lambda}$ gives

(2.35) $\varphi_2(x) = c_2 e^{i\sqrt{\lambda}\, x}$

as a solution, where c_2 is an arbitrary constant.

The general solution is the sum of the above solutions:

(2.36) $\varphi(x) = \varphi_1(x) + \varphi_2(x) = c_1 e^{-i\sqrt{\lambda}\, x} + c_2 e^{i\sqrt{\lambda}\, x}$

Apply Euler's identity

(2.37) $e^{\alpha + i\beta} = e^{\alpha}\,\mathrm{Cos}(\beta) + i\, e^{\alpha}\,\mathrm{Sin}(\beta)$ **:**

(2.38) $\varphi(x) = c_1\left(\mathrm{Cos}\left(\sqrt{\lambda}\, x\right) - i\,\mathrm{Sin}\left(\sqrt{\lambda}\, x\right)\right) + c_2\left(\mathrm{Cos}\left(\sqrt{\lambda}\, x\right) + i\,\mathrm{Sin}\left(\sqrt{\lambda}\, x\right)\right)$

Regroup terms:

(2.39) $\varphi(x) = (c_1 + c_2)\,\mathrm{Cos}\left(\sqrt{\lambda}\, x\right) + i(-c_1 + c_2)\,\mathrm{Sin}\left(\sqrt{\lambda}\, x\right)$

Redefine $c_1 + c_2$ as c_1 and $i(-c_1 + c_2)$ as c_2 since these are arbitrary constants, and we get:

(2.40) $\varphi(x) = c_1\,\mathrm{Cos}\left(\sqrt{\lambda}\, x\right) + c_2\,\mathrm{Sin}\left(\sqrt{\lambda}\, x\right)$

which is Eq. (A16) of Zhou, 2007. Considering the boundary condition at x=0, we get

(2.41 *a*) $\varphi(0) = c_1\,\mathrm{Cos}\left(\sqrt{\lambda}\, 0\right) + c_2\,\mathrm{Sin}\left(\sqrt{\lambda}\, 0\right) = 0$

(2.41 *b*) $c_1 = 0$

In order for $\varphi(0)$ to equal zero, both $c_1\mathrm{Cos}\left(\sqrt{\lambda}\,(0)\right)$ and $c_2\mathrm{Sin}\left(\sqrt{\lambda}\,(0)\right)$ must equal zero. The sine of zero equals zero, but the cosine of zero equals one; therefore, the only way for the cosine term to equal zero is for the coefficient c_1 to be zero.

Since we know that c_1=0, the solution Eq. (2.40) can be rewritten

(2.42) $\varphi(x) = c_2 \sin\sqrt{\lambda}\, x$

At x=L, the boundary condition Eq. (22.9b) requires

(2.43) $\frac{d}{dx}\left(c_2\,\mathrm{Sin}\sqrt{\lambda}\, L\right) = -\left(\frac{S\,J}{\mathrm{K}}\right) c_2\,\mathrm{Sin}\sqrt{\lambda}\, L$

The chain rule states that $\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$. To evaluate the LHS, use the chain rule and let u=$\sqrt{\lambda}\ L$ so that $\frac{du}{dx} = \sqrt{\lambda}$

(2.44) $\frac{d}{du}(c_2\ \mathrm{Sin}(u))\ \frac{du}{dx} = c_2\ \mathrm{Cos}(u)\left(\sqrt{\lambda}\right) = c_2\ \sqrt{\lambda}\ \mathrm{Cos}\ \sqrt{\lambda}\ L$

Now substitute Eq. (2.44) into the LHS of (2.43)

(2.45) $c_2\ \sqrt{\lambda}\ \mathrm{Cos}\ \sqrt{\lambda}\ L = -\left(\frac{S\,J}{\mathrm{K}}\right) c_2\ \mathrm{Sin}\ \sqrt{\lambda}\ L$

For simplicity in the calculation, define

(2.46) $h = \frac{S\,J}{\mathrm{K}}$

Dividing both sides of the Eq. (2.45) by -h c_2 and by Cos$\sqrt{\lambda}\ L$

$$\frac{c2\ \sqrt{\lambda}}{-h\ c2}\ \frac{\mathrm{Cos}\ \sqrt{\lambda}\ L}{\mathrm{Cos}\ \sqrt{\lambda}\ L} = \frac{-h\ c2}{-h\ c2}\ \frac{\mathrm{Sin}\ \sqrt{\lambda}\ L}{\mathrm{Cos}\ \sqrt{\lambda}\ L}$$

results in

(2.47) $\frac{\sqrt{\lambda}}{-h} = \frac{\mathrm{Sin}\ \sqrt{\lambda}\ L}{\mathrm{Cos}\ \sqrt{\lambda}\ L}$

which is equal to:

(2.48) $\mathrm{Tan}\ \sqrt{\lambda}\ L = -\frac{\sqrt{\lambda}}{h}$

The solution is now written as a sum of the eigenfunctions,

(2.49) $v(x,\ t) = \sum_{n=1}^{\infty} c_n(t)\ \varphi_n(x)$

where

(2.50) $\varphi_n(x) = \sin\ \sqrt{\lambda_n}\ x$

and the eigenvalues are given by solutions to Eq. (2.48).

The goal is now to calculate the coefficients $c_n(t)$. Recall from Eq. (2.14),

(2.14) $a\ \frac{\partial^2 v\,(x,\ t)}{\partial x^2} + Q = \frac{\partial v\,(x,\ t)}{\partial t}$

Substitute (2.49) into (2.14) to obtain (2.51):

(2.51) $\sum_{n=1}^{\infty} \frac{d\,c_n\,(t)}{dt}\ \varphi_n(x) = a \sum_{n=1}^{\infty} c_n(t)\ \frac{d^2\varphi_n\,(x)}{dx^2} + Q$

Because the eigenfunctions are orthogonal, we can apply Fourier’s Trick [7] to find a solution (The use of this method is justified in Appendix C.):

First, multiply by $\varphi_m\ (x)$:

(2.52) $\varphi_m(x) \sum_{n=1}^{\infty} \frac{d\,c_n\,(t)}{dt}\ \varphi_n(x) = a\ \varphi_m(x) \sum_{n=1}^{\infty} c_n(t)\ \frac{d^2\varphi_n\,(x)}{dx^2} + Q\ \varphi_m(x)$

Next, integrate from $\int_0^L dx$:

$$(2.53)\ \int_0^L \varphi_m(x) \sum_{n=1}^{\infty} \frac{d c_n(t)}{dt} \varphi_n(x)\, dx = a \int_0^L \varphi_m(x) \sum_{n=1}^{\infty} c_n(t) \frac{d^2 \varphi_n(x)}{dx^2}\, dx + Q \int_0^L \varphi_m(x)\, dx$$

Because the eigenfunctions, $\varphi_n(x) = \mathrm{Sin}\sqrt{\lambda_n}\, x$, are orthogonal,

$$(2.54)\ \int_0^L \varphi_m(x)\, \varphi_n(x)\, dx = \begin{cases} \int_0^L \varphi_m{}^2(x)\, dx & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}$$

Let $N = \int_0^L \varphi_m{}^2(x)\, dx$ be the normalization constant so that

$$(2.55)\ \frac{\int_0^L \varphi_m(x)\, \varphi_n(x)\, dx}{\int_0^L \varphi_m{}^2(x)\, dx} = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}$$

Dividing by N will yield orthonormal eigenfunctions and not merely orthogonal ones.

First, we will evaluate the term on the LHS:

$$(2.56)\ \int_0^L \varphi_m(x) \sum_{n=1}^{\infty} \frac{d c_n(t)}{dt} \varphi_n(x)\, dx$$

The only nonzero result for this term is when n=m, and that solution is:

$$(2.57)\ \frac{d c_m(t)}{dt} N$$

Next, we will evaluate the first term on the RHS:

$$(2.58)\ a \int_0^L \varphi_m(x) \sum_{n=1}^{\infty} c_n(t) \frac{d^2 \varphi_n(x)}{dx^2}\, dx$$

starting with the evaluation of the second derivative of $\varphi_n(x)$:

$$(2.59)\ \frac{d^2 \varphi_n(x)}{dx^2} = \frac{d^2}{dx^2}\left(\mathrm{Sin}\sqrt{\lambda_n}\, x\right) = \frac{d}{dx}\left(\frac{d}{dx}\left(\mathrm{Sin}\sqrt{\lambda_n}\, x\right)\right)$$

Let $u = \sqrt{\lambda_n}\, x$. Using the chain rule, $\frac{d}{dx}\left(\mathrm{Sin}\sqrt{\lambda_n}\, x\right)$ can be evaluated as :

$$(2.60)\ \frac{d}{du}\mathrm{Sin}(u)\, \frac{du}{dx} = \mathrm{Cos}(u)\sqrt{\lambda_n} = \sqrt{\lambda_n}\, \mathrm{Cos}\left(\sqrt{\lambda_n}\, x\right)$$

Replace $\frac{d}{dx}\left(\mathrm{Sin}\sqrt{\lambda_n}\, x\right)$ with the result we just found:

$$(2.61)\ \frac{d}{dx}\left(\frac{d}{dx}\left(\mathrm{Sin}\sqrt{\lambda_n}\, x\right)\right) = \frac{d}{dx}\left(\sqrt{\lambda_n}\, \mathrm{Cos}\left(\sqrt{\lambda_n}\, x\right)\right)$$

Again, let $u = \sqrt{\lambda_n}\, x$. Factor out the constant. Using the chain rule, $\sqrt{\lambda_n}\, \frac{d}{dx}\left(\mathrm{Cos}\left(\sqrt{\lambda_n}\, x\right)\right)$ can be evaluated as:

$$(2.62)\ \sqrt{\lambda_n}\, \frac{d}{du}\mathrm{Cos}(u)\, \frac{du}{dx} = \sqrt{\lambda_n}\left(-\mathrm{Sin}(u)\sqrt{\lambda_n}\right) = -\lambda_n\, \mathrm{Sin}\left(\sqrt{\lambda_n}\, x\right)$$

Now incorporate this result into the first term on the RHS:

$$(2.63\, a)\ a \int_0^L \varphi_m(x) \sum_{n=1}^{\infty} c_n(t)\, (-\lambda_n)\, \mathrm{Sin}\left(\sqrt{\lambda_n}\, x\right) dx$$

Additionally, we will replace $\text{Sin}\left(\sqrt{\lambda_n}\ x\right)$ with $\varphi_n(x)$ because they are equivalent, and it makes it easier to see how the expression can be simplified .

$$\textbf{(2.63 b)}\ a\int_0^L \varphi_m(x)\sum_{n=1}^{\infty} c_n(t)\ (-\lambda_n)\ \varphi_n(x)\,dx$$

Again, the only nonzero result for this term is when n=m, and that solution is:

$$\textbf{(2.64)}\ -a\,\lambda_m\,c_m(t)\,N$$

The second term on the RHS is:

$$\textbf{(2.65)}\ Q\int_0^L \varphi_m(x)\,dx$$

Putting together the results of evaluating all three terms yields:

$$\textbf{(2.66 a)}\ \frac{d\,c_m(t)}{d\,t}\,N = -a\,\lambda_m\,c_m(t)\,N + Q\int_0^L \varphi_m(x)\,dx$$

Rearranging this result yields:

$$\textbf{(2.66 b)}\ \frac{d\,c_m(t)}{d\,t}\,N + a\,\lambda_m\,c_m(t)\,N = Q\int_0^L \varphi_m(x)\,dx$$

Divide both sides by N, the normalization term:

$$\textbf{(2.66 c)}\ \frac{d\,c_m(t)}{d\,t} + a\,\lambda_m\,c_m(t) = \frac{Q\int_0^L \varphi_m(x)\,dx}{N}$$

Substitute the value $N=\int_0^L \varphi_m^2(x)\,dx$:

$$\textbf{(2.67)}\ \frac{d\,c_m(t)}{d\,t} + a\,\lambda_m\,c_m(t) = \frac{Q\int_0^L \varphi_m(x)\,dx}{\int_0^L \varphi^2{}_m(x)\,dx} = d_m$$

Evaluating the integral from the numerator of (2.67), I get:

$$\textbf{(2.68 a)}\ \int_0^L \varphi_m(x)\,dx = \int_0^L \text{Sin}\left(\sqrt{\lambda_m}\ x\right)dx = \frac{1}{\sqrt{\lambda_m}}\left(1-\text{Cos}\sqrt{\lambda_m}\ L\right)$$

Exploiting a rule for powers of trigonometric functions, $\text{Sin}^2 A = \frac{1}{2} - \frac{1}{2}\text{Cos}\ 2A$, which can be found in [8] Eq. (12.53), we will evaluate the integral from the denominator of Eq. (2.67):

$$\textbf{(2.68 b)}\ \int_0^L \varphi^2{}_m(x)\,dx = \int_0^L \text{Sin}^2\left(\sqrt{\lambda_m}\ x\right)dx = \int_0^L \frac{1-\text{Cos}\ 2\sqrt{\lambda_m}\ x}{2}\,dx =$$
$$\left(\int_0^L \frac{1}{2}\,dx - \frac{1}{2}\int_0^L \text{Cos}\ 2\sqrt{\lambda_m}\ x\,dx\right) = \frac{1}{2}\left(L - \frac{\text{Sin}\ 2\sqrt{\lambda_m}\ L}{2\sqrt{\lambda_m}}\right)$$

To get from the LHS to the RHS of the last line of Eq. (2.68b), we use formula (17.18.1) from [8]:

$$\int \cos ax\,dx = \frac{\sin ax}{a}$$

where $a=2\sqrt{\lambda_m}$.

Finally, to complete the problem, we incorporate the initial condition. At *t=0*, Eq. (2.49) becomes:

$$\textbf{(2.69)}\ v(x,\ 0) = \sum_{n=1}^{\infty} c_n(0)\,\varphi_n(x)$$

Because

$$\textbf{(2.18)}\ v(x,\ 0) = g(x)$$

we can equate the RHS of Eq. (2.69) with the RHS of Eq. (2.18):

$$\textbf{(2.70)}\ \sum_{n=1}^{\infty} c_n(0)\,\varphi_n(x) = g(x)$$

Again, Fourier's Trick [7] can be used. Multiply both sides by $\varphi_m(x)$ then integrate from $\int_0^L dx$:

$$\textbf{(2.71)}\ \int_0^L \varphi_m(x) \sum_{n=1}^{\infty} c_n(0)\,\varphi_n(x)\,dx = \int_0^L \varphi_m(x)\,g(x)\,dx$$

The only nonzero case is when n=m:

$$\textbf{(2.72)}\ c_m(0) \int_0^L \varphi_m{}^2(x)\,dx = \int_0^L \varphi_m(x)\,g(x)\,dx$$

Dividing both sides by $\int_0^L \varphi_m{}^2(x)\,dx$ yields:

$$\textbf{(2.73)}\ c_m(0) = \frac{\int_0^L \varphi_m(x)\,g(x)\,dx}{\int_0^L \varphi_m{}^2(x)\,dx}$$

We are now interested in solving for the term $c_m(t)$, and we will begin by using the following terms from Eq. (2.67):

$$\textbf{(2.74)}\ \frac{d\,c_m(t)}{dt} + a\,\lambda_m\,c_m(t) = d_m$$

because $d_m = \frac{Q \int_0^L \varphi_m(x)\,dx}{\int_0^L \varphi^2{}_m(x)\,dx}$ has already been evaluated.

(2.74) is of the form:

$$\textbf{(2.75)}\ y' + P(t)\,y = Q(t)$$

Note: This Q(t) is unrelated to the term Q in previous equations.

The technique used to solve Eq. (2.74) is to find an integrating factor.

In our differential equation, Eq. (2.74),

$$\textbf{(2.76)}\ y = c_m(t), \quad P(t) = a\,\lambda_m, \quad Q(t) = d_m$$

The integrating factor (IF) is:

$$\textbf{(2.77)}\ \mathrm{IF} = \exp\left[\int_0^t Q(t)\,dt\right] = \exp\left[\int_0^t a\,\lambda_m\,dt\right] = \exp[a\,\lambda_m\,t]$$

Now that we've found the IF, we'll multiply both sides of Eq. (2.74) by it:

$$\textbf{(2.78)}\ \frac{d\,c_m(t)}{dt}\,e^{a\,\lambda_m\,t} + a\ \lambda_m\,c_m(t)\,e^{a\,\lambda_m\,t} = d_m\,e^{a\,\lambda_m\,t}$$

The derivative of an exponential function has the form:

$$(2.79)\ \frac{d e^u}{d t} = e^u \frac{d u}{d t}$$

Rearranging the second term of the LHS of Eq. (2.78) reveals that is the derivative of an exponential function multiplied by $c_m(t)$:

$$(2.80)\ e^{a \lambda_m t}\, a\ \lambda_m\, c_m(t) = e^u \frac{d u}{d t}\, c_m(t)$$

where:

$$(2.81)\ u = a \lambda_m t, \quad e^u = e^{a \lambda_m t}, \quad \frac{d u}{d t} = a\ \lambda_m$$

Thus,

$$(2.82)\ e^u \frac{d u}{d t} = e^{a \lambda_m t} \frac{d (a \lambda_m t)}{d t} = e^{a \lambda_m t}\, a\ \lambda_m$$

The product rule for taking derivatives states:

$$(2.83)\ d(u\, v) = u\, d v + v\, d u$$

Further examination of the LHS of Eq. (2.78), reveals that it is the derivative of the product of $c_m(t)$ and $e^{a \lambda_m t}$where,

$$(2.84)\ u = e^{a \lambda_m t}, \quad v = c_m(t):$$

$$(2.85)\ \frac{d}{d t}\left(e^{a \lambda_m t}\, c_m(t)\right) = e^{a \lambda_m t} \frac{d c_m(t)}{d t} + c_m(t) \frac{d e^{a \lambda_m t}}{d t}$$
$$= e^{a \lambda_m t} \frac{d c_m(t)}{d t} + c_m(t)\, a\ \lambda_m\, e^{a \lambda_m t}$$

The last line should be recognizable as a rearrangement of the LHS of Eq. (2.78).

This serves to show that

$$(2.86)\ \frac{d}{d t}\left(e^{a \lambda_m t}\, c_m(t)\right) = d_m\, e^{a \lambda_m t}$$

Now that we’ve simplified things a bit, we’ll integrate from 0 to t with respect to time:

$$(2.87)\ \int_0^t \frac{d}{d t}\left(e^{a \lambda_m t}\, c_m(t)\right) d t = \int_0^t d_m\, e^{a \lambda_m t}\, d t$$

Evaluate the LHS first:

$$(2.88)\ \int_0^t \frac{d}{d t}\left(e^{a \lambda_m t}\, c_m(t)\right) d t = \left[c_m(t)\, e^{a \lambda_m t}\right]_0^t = c_m(t)\, e^{a \lambda_m t} - c_m(0)$$

Next, the RHS:

The formula for integrating an eponential of the form e^{ax}, which can be found in [8] Eq. (17.25.1) is:

$$\int e^{ax}\, d x = \frac{e^{ax}}{a}$$

This is suitable for evaluating our integral:

$$(2.89\ a)\ \int_0^t d_m\, e^{a \lambda_m t}\, d t$$

Factor out the constant:

$$\textbf{(2.89 b)}\ d_m \int_0^t e^{a\lambda_m t}\, dt$$

and substitue t=x and a$\lambda_m = a$ into Eq. (17.25.1).

The result is:

$$\textbf{(2.90)}\ d_m\left[\frac{e^{a\lambda_m t}}{a\lambda_m}\right]_0^t = d_m\left[\frac{e^{a\lambda_m t}}{a\lambda_m} - \frac{1}{a\lambda_m}\right] = \frac{d_m\, e^{a\lambda_m t}}{a\lambda_m} - \frac{d_m}{a\lambda_m}$$

Now equate the results of evaluating the LHS and the RHS:

$$\textbf{(2.91 a)}\ c_m(t)\, e^{a\lambda_m t} - c_m(0) = \frac{d_m\, e^{a\lambda_m t}}{a\lambda_m} - \frac{d_m}{a\lambda_m}$$

Rearrange this equation as follows:

$$\textbf{(2.91 b)}\ c_m(t)\, e^{a\lambda_m t} = c_m(0) - \frac{d_m}{a\lambda_m} + \frac{d_m\, e^{a\lambda_m t}}{a\lambda_m}$$

Now divide both sides by $e^{a\lambda_m t}$:

$$\textbf{(2.91 c)}\ c_m(t) = \left(c_m(0) - \frac{d_m}{a\lambda_m}\right) e^{-a\lambda_m t} + \frac{d_m}{a\lambda_m}$$

We will replace $c_m(0)$ with the value that we found earlier:

$$\textbf{(2.73)}\ c_m(0) = \frac{\int_0^L \varphi_m(x)\, g(x)\, dx}{\int_0^L \varphi_m{}^2(x)\, dx}$$

Returning to the generic subscript n, we arrive at a solution for $c_n(t)$:

$$\textbf{(2.92)}\ c_n(t) = \left(\frac{\int_0^L \varphi_n(x)\, g(x)\, dx}{\int_0^L \varphi_n{}^2(x)\, dx} - \frac{d_n}{a\lambda_n}\right) e^{-a\lambda_n t} + \frac{d_n}{a\lambda_n}$$

This solution, Eq. (2.92), along with the solution to Eq. (2.50), is incorporated into Eq. (2.49) to complete the transient solution. Then the completed transient solution, v(x,t), along with the steady-state solution, r(x), can be substituted into the rearranged form of Eq. (2.6) to yield the complete solution to Eq. (2.1).

$$\textbf{(2.6)}\ T(x, t) = r(x) + v(x, t)$$

$$\textbf{(2.93)}\ T(x, t) = r(x) + \sum_{n=1}^{\infty} c_n(t)\, \varphi_n(x)$$

Finally, the solution for T(x,t) is

$$\textbf{(2.94)}\ T(x, t) = T_h\left(1 - \frac{x}{L}\right)^2 + \sum_{n=1}^{\infty} c_n(t)\, \text{Sin}\sqrt{\lambda_n}\ (x)$$

Compare this to Eq. (A26) in[1], where the boundaries are flipped (the heat sink is at $x = L$),

$$\textbf{(A26)}\ T(x, t) = \frac{T_h\, x^2}{L^2} + \sum_{n=1}^{\infty} c_n(t)\, \text{Sin}\sqrt{\lambda_n}\ (L - x)$$

3. Numerical Calculation

3.A Procedure

To perform calculations using the results of this derivation, the first step is to determine the parameters of the system from experiment or literature references and establish numerical values for Q and h. Here, we will use values from [1]. The eigenvalues depend on the Seebeck coefficient (S), the current density (J), the thermal conductivity (K), and the length of the sample (L). Once these are determined, the $c_n(0)$ can be determined from the initial conditions - the temperature profile, *T(x,0)*, or the auxiliary temperature profile $g(x)$.

Calculation of the temperature as a function of time and distance along the thermoelectric element proceeds as follows. The temperature is given by the eigenfunction expansion Eq. (2.94)

$$\textbf{(2.94)}\ T(x,\,t) = T_h\left(1 - \frac{x}{L}\right)^2 + \sum_{n=1}^{\infty} c_n(t)\,\varphi_n(x)$$

with eigenfunctions

$$\textbf{(2.50)}\ \varphi_n(x) = \sin\left(\sqrt{\lambda_n}\ x\right).$$

The set of eigenvalues are given by the solutions to Eq. (2.48)

$$\textbf{(2.48)}\ \tan\sqrt{\lambda_n}\ L = -\frac{\sqrt{\lambda_n}}{h}$$

The coefficients c_n are given by Eq. (2.91c) returned to the generic subscript *n:*

$$\textbf{(2.91 c)}\ c_n(t) = \left(c_n(0) - \frac{d_n}{a\,\lambda_n}\right) e^{-a\,\lambda_n\,t} + \frac{d_n}{a\,\lambda_n}$$

with initial condition Eq. (2.73) again with the generic subscript *n*:

$$\textbf{(2.73)}\ c_n(0) = \frac{\int_0^L \varphi_n(x)\,g(x)\,dx}{\int_0^L \varphi_n{}^2(x)\,dx}$$

where

$$\textbf{(2.20)}\ g(x) = T_h\left(\frac{2\,x}{L} - \frac{x^2}{L^2}\right)$$

The constant d_n is given by Eq. (2.67) again with the generic subscript *n*:

$$\textbf{(2.67)}\ d_n = \frac{Q\int_0^L \varphi_n(x)\,dx}{\int_0^L \varphi^2{}_n(x)\,dx}$$

and the parameter Q is

$$\textbf{(2.15)}\ Q = \frac{2\,a\,T_h}{L^2} + \frac{J^2\,a}{\mathrm{K}\,\sigma}$$

■ 3.B Typical Values

For the calculations, typical values of the material parameters are taken from Zhou, 2007 [1]

S=220 μV/K

K=1.83 W/m-K

$\sigma = 1.17 \times 10^5\ \Omega^{-1}\ m^{-1}$

The geometrical parameters for the thermoelectric element are

L=10 mm

w=2 mm

d=2 mm

The calculations will be given for an applied current of 3 A.

■ 3.C Results

The simulation is run over the course of three minutes. Each plot shows the temperature profile at a given point along the length of the sample. The *Mathematica* code used to arrive at these results is located in Appendix B.

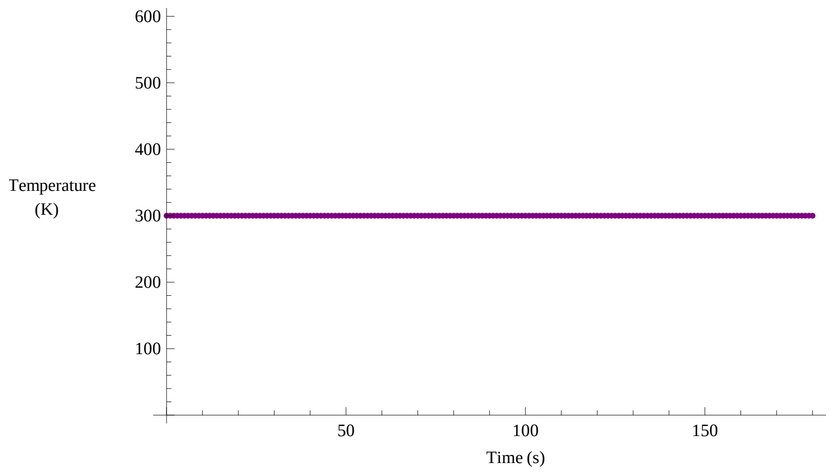

Figure 2. Temperature as a function of time at *u=0*.

At the hot side of the sample, which is in contact with the heat sink (where *u=0*), the temperature starts out at 300 K and stays stable at 300 K for the duration of the system's operation because it is in contact with the heat sink.

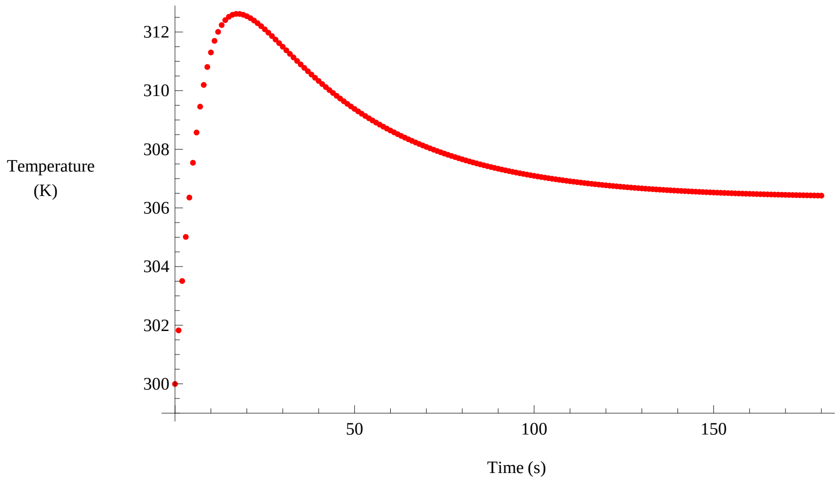

Figure 3. Temperature as a function of time at *u=0.25*.

One quarter of the way down the sample from the heat sink, where *u=0.25*, the initial temperature is 299.995 K. After turning the system on, it heats up reaching 312.618 K after 17 seconds of operation. After that it begins to cool reaching 306.536 K after 180 seconds of operation.

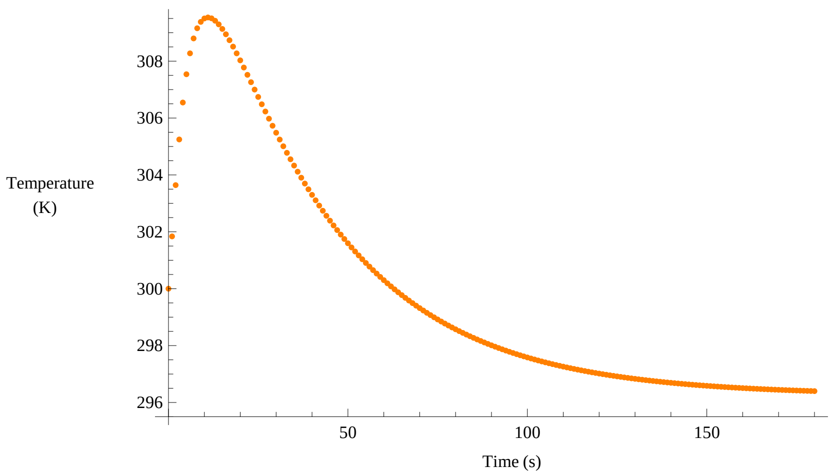

Figure 4. Temperature as a function of time at *u=0.50*

In the middle of the sample, where *u=0.50*, the initial temperature is 300.000 K. When the system is turned on, the temperature rises at first reaching 309.536 K after 11 seconds, then it begins cooling. The temperaure after 180 seconds of operation is 296.399 K.

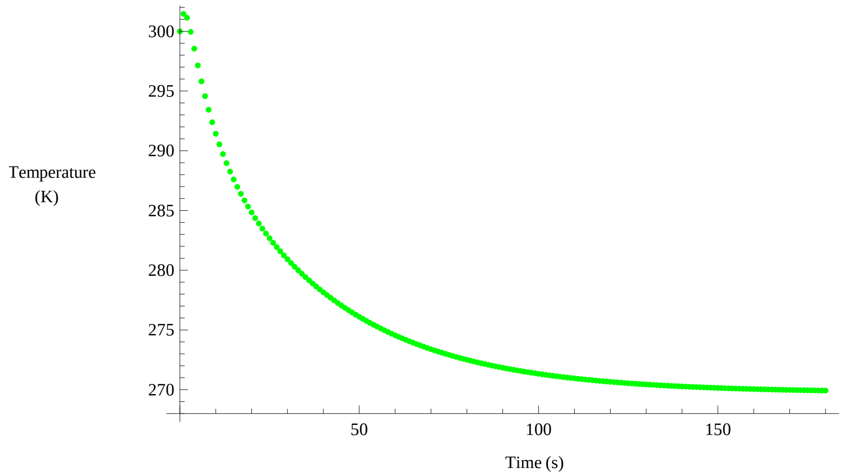

Figure 5. Temperature as a function of time at *u=0.75*.

Three quarters of the way down the sample from the heat sink, where *u=0.75*, the temperature stars out at 299.989 K. It heats up a tiny bit to 301.453 K after one second of operation, but the temperature starts dropping after that and reaches 269.925 K after 180 seconds of operation.

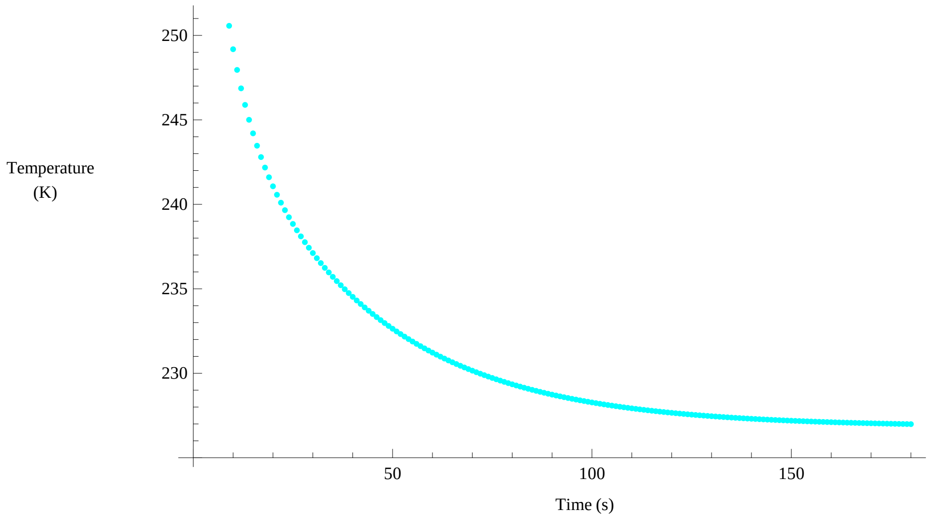

Figure 6. Temperature as a function of time at *u=1.00*.

At the cold end of the sample, where *u=1.00*, the initial temperature is 299.452 K. When the system is turned on, the temperature drops continuously and reaches a final temperature of 226.989 K after 180 seconds.

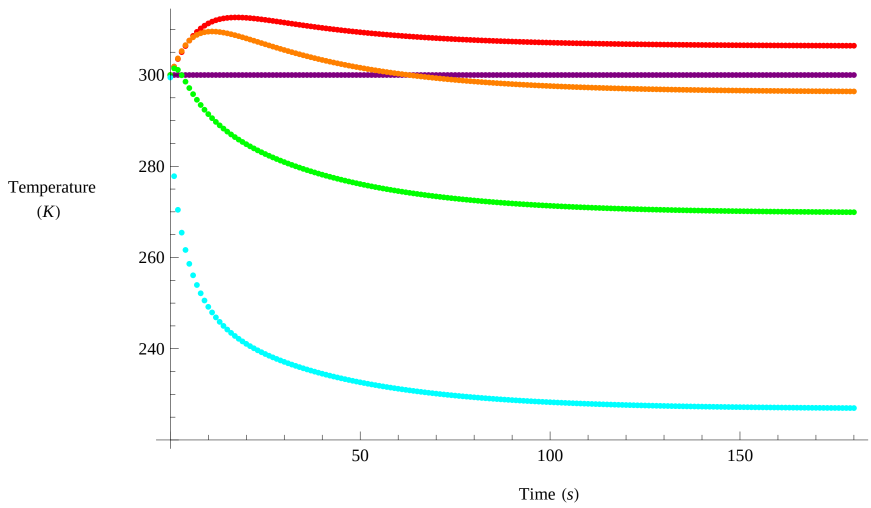

Figure 7. Temperature as a function of time at *u=0, u=0.25, u=0.50, u=0.75,* and *u=1.00*.

The temperature profiles for each position where temperature was measured appear together on this graph so the reader can compare what occurred at each measured point along the length of the sample during the experiment.

4. References

[1] Q. Zhou, Z. Bian, and A. Shakouri, "Pulsed cooling of inhomogeneous thermoelectric materials," Journal of Physics D: Applied Physics 40, pp. 4376-4382, 2007. http://dx.doi.org/10.1088/0022-3727/40/14/037.

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[3] R. Yang, G. Chen, A. Ravi Kumar, G. J. Snyder, and J.-P. Fleurial, "Transient cooling of ther moelectriccoolers and its applications for microdevices," Energy Conversion and Management 46, pp. 1407-1421, 2005. http://dx.doi.org/10.1016/j.encon man.2004.07.004.

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[8] M. R. Spiegel, S. Lipschutz, and J. Liu, Schaum's Outline of Mathematical Handbook of Formulas and Tables, 3rd Edition. New York: McGraw-Hill, 2009.

[9] P. Garrity, "Alternative Energy Production Through Thermoelectrics," Powerpoint lecture presented in SCI 1053 on the University of New Orleans campus on October 5th, 2011.

5. Appendix

▪ Appendix A

Numerical Solution to the Eigenvalue Equation Using *Mathematica*

The eigenvalues, λ_n, are given by the solution to:

(2.95) $\tan(z_n) = -\frac{z_n}{h\,L}$

Eq. (2.95) is simply Eq. (2.48) where

(2.96) $\sqrt{\lambda_n}\;L = z_n$

and

(2.46) $h = \frac{S\,J}{\mathrm{K}}$

What we are solving for are the eigenvalues of the homogeneous PDE Eq. (2.21). The other equations in this paper can be done analytically; however, to determine the roots of this equation, the only option is to solve numerically.

In order to do this, we will use the Mathematica function FindRoot[], which has the form:

```
FindRoot[lhs == rhs, {x, x0}]
```

Using this command means that we will be given the value when the LHS of the equation is equal to the RHS in the range from x to x0. The values where they agree (LHS=RHS) are solutions to the equation.

To visualize this, we can plot $f_1(z)$ =Tan(z) and $f_2(z)=-\frac{z}{h\,L}$. Solutions are where the two functions intersect. Since the tangent function is periodic, we will see one solution in each period.

In order to do this for our equation, we will assign h and L a value.

```
J = I / w^2 = 3.0 / (2 × 10^-3)^2 = 750 × 10^3 A / m^2
h0 = (220 × 10^-6) (750 × 10^3 ) / 1.83
```

```
90.1639
```

```
eqEV = Tan[z] == -z/(L h) /. {L → 10^-3, h → h0}
```

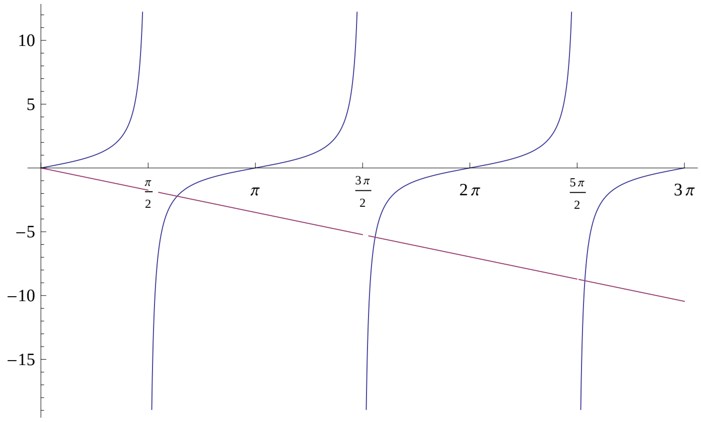
```
Tan[z] == -1.10909 z
```

```
f1[z_] = Tan[z]
f2[z_] = -1.10909 z
```

```
Tan[z]
```

```
-1.10909 z
```

```
Plot[{f1[z], f2[z]}, {z, 0, 3 π}, Exclusions → {Cos[z] == 0},
 Ticks → {{0, π / 2, π, 3 π / 2, 2 π, 5 π / 2, 3 π}, Automatic}]
```



Notice that Tan(z) is less than zero when $\frac{\pi}{2}$<x<π, $\frac{3\pi}{2}$<x<2π, $\frac{5\pi}{2}$<x<3π, ...

These are the only regions where $f_1(z)$ and $f_2(z)$ could possibly intersect because $f_2(z)$ is always less than zero. Again, notice that there is exactly one solution in each of these regions; therefore, we will command the program to start looking for solutions at points a little larger than $\frac{\pi}{2}$, $\frac{3\pi}{2}$, $\frac{5\pi}{2}$, ... and hope that they converge to the solution.

Since we will compute many values for λ, and we will want to operate on them all, we will put them into an array, λ={}.

Notice that in the Mathematica code below, that although we have been operating with z=$\sqrt{\lambda}$ L, to fill the array, we append to the array an expression in terms of znew that is equal to λ:

(znew is just z that has been replaced by sol1, which is the value of z within a particular range.)

$$\frac{\text{znew}^2}{L^2} \Longrightarrow \frac{\left(\sqrt{\lambda}\ L\right)^2}{L^2} = \frac{\left(\sqrt{\lambda}\right)^2 L^2}{L^2} = \left(\sqrt{\lambda}\right)^2 = \lambda$$

```
λ = {};
For[i = 1, i <= 100, i++,
  sol1 = FindRoot[eqEV, {z, (i - 1 / 2) π + 0.1}];
  znew = z /. sol1;
  zapprox = (i - 1. / 2.) π;
  AppendTo[λ, znew² / L²]];
```

The results of this calculation are available in the Appendix D. Since we see that it does converge, once the first 100 or so solutions are calculated, we can switch to the approximate solution:

$$\text{zapprox} = \pi \left(i - \frac{1.}{2.}\right)$$

Appendix B

Calculation of T(x,t) and Plots Using *Mathematica*

Input Parameters

This sets all the input parameters.

```
L = 10. × 10^-3 (* Length of the sample *)
current = 3.0 (* Input current*)
K = 1.83 (* Thermal conductivity (capital KAPPA) *)
S = 220 × 10^-6 (* Seebeck coefficient *)
σ = 1.17 × 10^5 (* Electrical conductivity *)
a = 0.7 × 10^-6 (* Thermal diffusivity *)
w = 2 × 10^-3 (* Width of the sample, area is w^2 *)
Th = 300 (* Heat sink temperature *)
```

```
0.01
3.
1.83
```

$\frac{11}{50000}$

```
117000.
```

$7. \times 10^{-7}$

$\frac{1}{500}$

```
300
```

Derived Parameters

```
J = current / w^2 (* Current density *)
h = S J / K
```

$Q = \frac{2\,a\,Th}{L^2} + \frac{J^2\,a}{K\,\sigma}$ `(* Eq. (15) *)`

```
750000.
90.1639
6.03901
```

Lists

Functions have [], but lists (arrays) have double brackets [[n]].

These are all the lists for the entire numerical calculation:

z - eigenvalues (actually, $\sqrt{\lambda}\,L$)

d - Eq. (67)

c0 - Eq. (73)

c - Eq. (91 c)

α - used to calculated c (α = a λ)

T1 - Eq. (94) with u = 0.0

T2 - Eq. (94) with u = 0.25

T3 - Eq. (94) with u = 0.5

T4 - Eq. (94) with u = 0.75

T5 - Eq. (94) with u = 1.0

All lists are initiallized with {} as in z={}

```
eqEV = Tan[zn] == -zn / (h L)
Tan[zn] == -1.10909 zn
```

Use the numerical root finder to calculate the first 100 eigenvalues.

```
z = {};
For[n = 1, n <= 100, n++,
 solEV = FindRoot[eqEV, {zn, (n - 1 / 2) π + 0.1}];
 AppendTo[z, zn /. solEV];
]
```

Use the approximation to find the next 900 values.

```
For[n = 101, n <= 1000, n++,
 zapprox = π (n - 1./2.);
 zn = zapprox;
 AppendTo[z, zn ];
]
```

- **d_n, $C_n(0)$**

```
d = {};
c0 = {};
α = {};
For[n = 1, n <= 100, n++,
  (* Intϕ = ∫_0^1 Sin[z[[n]] u] du *)
  (* Once evaluated, the integral equals: *)
  Intϕ = (1 - Cos[z[[n]]]) / z[[n]];
  (* IntϕSQ = ∫_0^1 Sin[z[[n]] u]^2 du *)
  (* Once evaluated, the integral equals: *)
  IntϕSQ = 1/2 - Sin[2 z[[n]]] / (4 z[[n]]);
  dn = Q Intϕ / IntϕSQ;
  AppendTo[d, dn];
  (* Intgϕ = Th ∫_0^1 (2u-u^2) Sin[z[[n]] u] du *)
  (* Once evaluated, the integral equals: *)
  Intgϕ = Th (2 - (2 + z[[n]]^2) Cos[z[[n]]]) / z[[n]]^3;
  cn0 = Intgϕ / IntϕSQ;
  AppendTo[c0, cn0];
  αn = a z[[n]]^2 / L^2;
  AppendTo[α, αn];
]
```

- **$C_n(t)$**

```
Clear[t]
c = {};
For[n = 1, n ≤ 100, n++,
  cn = (c0[[n]] - d[[n]] / α[[n]]) e^(-α[[n]] t) + d[[n]] / α[[n]];
  AppendTo[c, cn];
]
```

Final Solution

```
T1 = {};
u = 0.0;
For[t = 0, t ≤ 180, t = t + 1,

 For[vsum = 0; n = 1, n <= 100, n++,
  vsum = vsum + c[[n]] Sin[z[[n]] u]
 ];

 T0 = Th (1 - u)^2 + vsum;
 AppendTo[T1, {t, T0}];
]
T2 = {};
u = 0.25;
For[t = 0, t ≤ 180, t = t + 1,

 For[vsum = 0; n = 1, n <= 100, n++,
  vsum = vsum + c[[n]] Sin[z[[n]] u]
 ];

 T0 = Th (1 - u)^2 + vsum;
 AppendTo[T2, {t, T0}];
]
T3 = {};
u = 0.5;
For[t = 0, t ≤ 180, t = t + 1,

 For[vsum = 0; n = 1, n <= 100, n++,
  vsum = vsum + c[[n]] Sin[z[[n]] u]
 ];
 T0 = Th (1 - u)^2 + vsum;
 AppendTo[T3, {t, T0}];
]
```

```
T4 = {};
u = 0.75;
For[t = 0, t ≤ 180, t = t + 1,

 For[vsum = 0; n = 1, n <= 100, n++,
  vsum = vsum + c[[n]] Sin[z[[n]] u]
 ];

 T0 = Th (1 - u)^2 + vsum;
 AppendTo[T4, {t, T0}];
]
T5 = {};
u = 1.0;
For[t = 0, t ≤ 180, t = t + 1,

 For[vsum = 0; n = 1, n <= 100, n++,
  vsum = vsum + c[[n]] Sin[z[[n]] u]
 ];

 T0 = Th (1 - u)^2 + vsum;
 AppendTo[T5, {t, T0}];
]
```

■ Plots

```
ListPlot[T1]

ListPlot[T2]

ListPlot[T3]

ListPlot[T4]

ListPlot[T5]

ListPlot[{T1, T2, T3, T4, T5}]
```

■ Appendix C

Proof of the Orthogonality of the Eigenfunctions

Two functions φ_m and φ_n are orthogonal if their inner product $\langle\varphi_m,\varphi_n\rangle$ is equal to zero for $m \neq n$. In our case, the inner product is defined as:

$$(C.1)\quad \langle\varphi_m, \varphi_n\rangle = \int \varphi_m{}^* (x)\, \varphi_n (x)\, dx$$

The asterisk denotes the complex conjugate of the function φ_m, and since φ_m has no imaginary parts, the complex conjugate is just the function itself.

Two techniques that we used, namely the eigenfunction expansion method and Fourier's Trick, rely on the orthogonality of the eigenfunctions in order to produce valid results. The following is verification that the eigenfunctions are, in fact, orthogonal:

$$(C.2)\ \int_0^L \varphi_m(x)\,\varphi_n(x)\,dx = \int_0^L \mathrm{Sin}\left(\sqrt{\lambda_m}\,x\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\,x\right)dx$$

Using a relationship for the product of trigonometric functions:

$$(C.3)\ \mathrm{Sin}(A)\,\mathrm{Sin}(B) = \frac{1}{2}\{\mathrm{Cos}(A-B) - \mathrm{Cos}(A+B)\}$$

$$(C.4)\ \int_0^L \mathrm{Sin}\left(\sqrt{\lambda_m}\,x\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\,x\right)dx =$$

$$\frac{1}{2}\int_0^L\left\{\mathrm{Cos}\left[\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)x\right]-\mathrm{Cos}\left[\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)x\right]\right\}dx$$

The formula for this integral, Eq. 17.18.1 in Schaum's [8] is:

$$(17.18\ .1)\ \int \mathrm{Cos}\,\alpha x\,dx = \frac{\mathrm{Sin}\,\alpha x}{\alpha}$$

where

$$\alpha = \left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)$$

So the above integral is equal to:

$$(C.5)\ \frac{1}{2}\left(\frac{\mathrm{Sin}\left[\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)x\right]}{\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)}-\frac{\mathrm{Sin}\left[\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)x\right]}{\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)}\right|_0^L =$$

$$\frac{\mathrm{Sin}\left[\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)L\right]}{2\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)}-\frac{\mathrm{Sin}\left[\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)L\right]}{2\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)}$$

Using an addition formula for trigonometric functions, which is Eq. 12.34 in [8]:

$$(12.34)\ \mathrm{Sin}(A\pm B) = \mathrm{Sin}(A)\,\mathrm{Cos}(B)\pm\mathrm{Cos}(A)\,\mathrm{Sin}(B)$$

where

$$A = \sqrt{\lambda_m}\,L,\quad B = \sqrt{\lambda_n}\,L$$

$$(C.6)\ \frac{\mathrm{Sin}\left[\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)L\right]}{\left(2\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)\right)}-\frac{\mathrm{Sin}\left[\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)L\right]}{\left(2\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)\right)} =$$

$$\left(\mathrm{Sin}\left(\sqrt{\lambda_m}\,L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\,L\right)-\mathrm{Cos}\left(\sqrt{\lambda_m}\,L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\,L\right)\right)\Big/\left(2\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)\right)-$$
$$\left(\mathrm{Sin}\left(\sqrt{\lambda_m}\,L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\,L\right)+\mathrm{Cos}\left(\sqrt{\lambda_m}\,L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\,L\right)\right)\Big/\left(2\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)\right)$$

To get these to have the same denominator, multiply the first term by $\frac{\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)}{\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)}$ and the second term by $\frac{\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)}{\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)}$.

The result is:

$$(C.7)\ \left(\mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\ L\right)-\mathrm{Cos}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)\right)\Big/\left(2\left(\lambda_m-\lambda_n\right)\right)\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)-\left(\mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\ L\right)+\mathrm{Cos}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)\right)\Big/\left(2\left(\lambda_m-\lambda_n\right)\right)\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)$$

I will factor out the $\frac{1}{2(\lambda_m-\lambda_n)}$ and distribute the $\left(\sqrt{\lambda_m}+\sqrt{\lambda_n}\right)$ in the first term and the $\left(\sqrt{\lambda_m}-\sqrt{\lambda_n}\right)$ in the second term:

$$(C.8)\ \frac{1}{2\left(\lambda_m-\lambda_n\right)}\Big\{\sqrt{\lambda_m}\ \mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\ L\right)-\sqrt{\lambda_m}\ \mathrm{Cos}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)+\sqrt{\lambda_n}\ \mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\ L\right)-\sqrt{\lambda_n}\ \mathrm{Cos}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)-\sqrt{\lambda_m}\ \mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\ L\right)-\sqrt{\lambda_m}\ \mathrm{Cos}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)+\sqrt{\lambda_n}\ \mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\ L\right)+\sqrt{\lambda_n}\ \mathrm{Cos}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)\Big\}$$

Some of the terms cancel and some combine leaving us with:

$$(C.9)\ \frac{1}{2\left(\lambda_m-\lambda_n\right)}\left\{2\sqrt{\lambda_n}\ \mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\ L\right)-2\sqrt{\lambda_m}\ \mathrm{Cos}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)\right\}=\frac{1}{\left(\lambda_m-\lambda_n\right)}\left\{\sqrt{\lambda_n}\ \mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\ L\right)-\sqrt{\lambda_m}\ \mathrm{Cos}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)\right\}$$

Therefore,

$$\int_0^L \mathrm{Sin}\left(\sqrt{\lambda_m}\ x\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ x\right)dx=\frac{1}{\left(\lambda_m-\lambda_n\right)}\left\{\sqrt{\lambda_n}\ \mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Cos}\left(\sqrt{\lambda_n}\ L\right)-\sqrt{\lambda_m}\ \mathrm{Cos}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)\right\}\quad (C.10)$$

From Eq. (2.47),

$$(2.47)\ \frac{\sqrt{\lambda}}{-h}=\frac{\mathrm{Sin}\sqrt{\lambda}\ L}{\mathrm{Cos}\sqrt{\lambda}\ L}$$

so rearranging this shows that

$$(C.11a)\ \mathrm{Cos}\sqrt{\lambda_m}\ L=\frac{-h}{\sqrt{\lambda_m}}\mathrm{Sin}\sqrt{\lambda_m}\ L$$

and

$$(C.11b)\ \mathrm{Cos}\sqrt{\lambda_n}\ L=\frac{-h}{\sqrt{\lambda_n}}\mathrm{Sin}\sqrt{\lambda_n}\ L$$

Make these substitutions for $\mathrm{Cos}\sqrt{\lambda_m}\ L$ and $\mathrm{Cos}\sqrt{\lambda_n}\ L$:

$$(C.12)\ \frac{1}{\left(\lambda_m-\lambda_n\right)}\left\{\sqrt{\lambda_n}\ \mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\frac{-h}{\sqrt{\lambda_n}}\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)-\sqrt{\lambda_m}\ \frac{-h}{\sqrt{\lambda_m}}\mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)\right\}=$$

$$\frac{-h}{\left(\lambda_m-\lambda_n\right)}\left\{\mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)-\mathrm{Sin}\left(\sqrt{\lambda_m}\ L\right)\mathrm{Sin}\left(\sqrt{\lambda_n}\ L\right)\right\}=0$$

for $n \neq m$, the answer is, in fact, zero. For $n=m$ this form is indeterminate, but we can simply return to the integral

$$\int_0^L \varphi_m(x)\,\varphi_n(x)\,dx = \int_0^L \varphi_m(x)\,\varphi_m(x)\,dx = \int_0^L \mathrm{Sin}^2\left(\sqrt{\lambda_m}\,x\right) dx \qquad (C.13)$$

This justifies our use of the eigenfunction expansion method and Fourier's Trick and supports their validity.

Appendix D

List of the First 100 Calculated Eigenvalues and Their Approximated Values

The results of calculating λ_n, the eigenvalues of Eq. (21)

```
λ = {};
For[i = 1, i <= 100, i++,
 sol1 = FindRoot[eqEV, {zn, (i - 1 / 2) π + 0.1}];
 znew = zn /. sol1;
 zapprox = (i - 1. / 2.) π;
 AppendTo[λ, znew^2 / L^2];
 Print[i, ": ", znew, " - ", zapprox]]
```

```
1: 1.99523 - 1.5708
2: 4.89456 - 4.71239
3: 7.96668 - 7.85398
4: 11.0768 - 10.9956
5: 14.2006 - 14.1372
6: 17.3307 - 17.2788
7: 20.4644 - 20.4204
8: 23.6001 - 23.5619
9: 26.7372 - 26.7035
10: 29.8753 - 29.8451
11: 33.014 - 32.9867
12: 36.1532 - 36.1283
13: 39.2929 - 39.2699
14: 42.4327 - 42.4115
15: 45.5729 - 45.5531
16: 48.7132 - 48.6947
17: 51.8537 - 51.8363
18: 54.9943 - 54.9779
19: 58.135 - 58.1195
```

20: 61.2758 – 61.2611

21: 64.4166 – 64.4026

22: 67.5576 – 67.5442

23: 70.6986 – 70.6858

24: 73.8396 – 73.8274

25: 76.9807 – 76.969

26: 80.1219 – 80.1106

27: 83.263 – 83.2522

28: 86.4042 – 86.3938

29: 89.5455 – 89.5354

30: 92.6867 – 92.677

31: 95.828 – 95.8186

32: 98.9693 – 98.9602

33: 102.111 – 102.102

34: 105.252 – 105.243

35: 108.393 – 108.385

36: 111.535 – 111.527

37: 114.676 – 114.668

38: 117.817 – 117.81

39: 120.959 – 120.951

40: 124.1 – 124.093

41: 127.242 – 127.235

42: 130.383 – 130.376

43: 133.524 – 133.518

44: 136.666 – 136.659

45: 139.807 – 139.801

46: 142.949 – 142.942

47: 146.09 – 146.084

48: 149.232 – 149.226

49: 152.373 – 152.367

50: 155.515 – 155.509

51: 158.656 – 158.65

52: 161.798 – 161.792

53: 164.939 – 164.934

54: 168.081 – 168.075

55: 171.222 – 171.217

56: 174.364 – 174.358

57: 177.505 – 177.5

58: 180.647 – 180.642

59: 183.788 – 183.783

60: 186.93 – 186.925

61: 190.071 – 190.066

62: 193.213 – 193.208

63: 196.354 – 196.35

64: 199.496 – 199.491

65: 202.637 – 202.633

66: 205.779 – 205.774

67: 208.92 – 208.916

68: 212.062 – 212.058

69: 215.203 – 215.199

70: 218.345 – 218.341

71: 221.486 – 221.482

72: 224.628 – 224.624

73: 227.769 – 227.765

74: 230.911 – 230.907

75: 234.053 – 234.049

76: 237.194 – 237.19

77: 240.336 – 240.332

78: 243.477 – 243.473

79: 246.619 – 246.615

80: 249.76 – 249.757

81: 252.902 – 252.898

82: 256.043 – 256.04

83: 259.185 – 259.181

84: 262.326 – 262.323

85: 265.468 – 265.465

86: 268.61 – 268.606

87: 271.751 – 271.748

88: 274.893 – 274.889

89: 278.034 – 278.031

90: 281.176 – 281.173

91: 284.317 – 284.314

92: 287.459 – 287.456

93: 290.6 – 290.597

94: 290.6 – 293.739

95: 293.742 – 296.881

96: 296.884 – 300.022

97: 300.025 – 303.164

98: 306.308 – 306.305

99: 309.45 – 309.447

100: 312.591 – 312.588

APPROVAL SHEET

This is to certify that Sunni Ann Siqueira has successfully completed her Senior Honors Thesis, entitled:

Calculation of Time-Dependent Heat Flow in a Thermoelectric Sample

Kevin L. Stokes — Director of Thesis

Juliette W. Ioup — for the Department

Carl D. Malmgren — for the University Honors Program

May 2, 2012
Date